

Tier 1 *In Vitro* Toxicokinetic Assays

Endpoint of Interest	NTP	EPA	
		National Center for Computational Toxicology (NCCT)	National Health and Environmental Effects Research Laboratory (NHEERL)
Hepatic Clearance	Human primary hepatocyte clearance		
Plasma Protein Binding			Ultracentrifugation assay
Renal Transport	Renal proximal tubule permeability assay		
Enterohepatic Recirculation		Piloting hepatic transporter assay	
<i>In Vitro</i> Disposition	Cell vs. nominal concentration (Tox21 joint project)	Cell vs. nominal concentration (Tox21 joint project)	

ECOS-EPA PFAS Call

October 30, 2017

4:00-5:00 pm ET

Call-in number: Conference Line / Ex. 6 code Personal Phone / Ex. 6

Webinar link: **Personal Matters / Ex. 6**

Agenda

1. Welcome and Introductions – Jennifer Orme-Zavaleta, EPA’s Office of Research and Development (ORD) (5 mins)
2. Amended TSCA: How implementation could influence actions around PFAS – Jeff Morris, Director, EPA’s Office of Pollution Prevention and Toxics (15 mins)
3. GenX in the Cape Fear River Basin
 - State update – Sheila Holman, NC DEQ Assistant Secretary for Environment (10 mins)
 - PFAS methods work to support NC – Tim Buckley, EPA ORD National Exposure Research Laboratory (5 mins)
4. Overview of the PFAS Investigation at Wright-Patterson AFB
 - Including the sampling of a sentinel well network designed to detect contamination before it impacts the city of Dayton’s downgradient wellfields – Bonnie Buthker, Chief, Southwest District Office, Ohio EPA (10 mins)
5. Ohio EPA Progress on Analytical Methods
 - Drinking water and direct injection method for other waters – Nik Dzamov, Chief, Division of Environmental Services, Ohio EPA (5 mins)
6. Updates from the EPA PFAS Workgroups
 - Methods Development – Chris Impellitteri, EPA ORD Co-Chair (5 mins)
 - Toxicity – Lynn Flowers, EPA ORD Co-Chair (5 mins)
7. Open forum to share info (states)
8. Wrap-up and Adjourn – Jennifer Orme-Zavaleta, EPA ORD

Organizer: Matthews, Lisa[Matthews.Lisa@epa.gov]
From: Matthews, Lisa
Location:

Conference Line / Ex. 6

Code

Personal Phone / Ex. 6

 please register for webinar below
Importance: Normal
Subject: EPA-ECOS PFAS Call (updated)
Categories: important external meeting
Start Time: Mon 8/7/2017 8:00:00 PM
End Time: Mon 8/7/2017 9:00:00 PM
Required Attendees: kristy.richardson@state.co.us; Nicole Lugli; robert.kaliszewski@ct.gov; kerri.malinowski@maine.gov; douglas.fine@state.ma.us; c.mark.smith@state.ma.us; delaneyr@michigan.gov; krukowskim@michigan.gov; remusm@michigan.gov; clark.freise@des.nh.gov; Brandon.kernen@des.nh.gov; Steve.Maybury@dep.nj.gov; eileen.murphy@dec.ny.gov; robert.schick@dec.ny.gov; jason.fagel@dec.ny.gov; Holman, Sheila; linda.culpepper@ncdenr.gov; craig.butler@epa.ohio.gov; nik.dzamorov@epa.ohio.gov; susan.kessler@epa.ohio.gov; jenyfer.allen@epa.ohio.gov; MASTERSON.Kevin@deq.state.or.us; marz.nicole@deq.state.or.us; steven.jetter@state.or.us; Heidi.Hales@vermont.gov; Chuck Schwer; kzar461@ecy.wa.gov; janice.willey@navy.mil; aroberson@asdwa.org; chanson@ecos.org; slongsworth@ecos.org; Bowe, Patrick; Iwenofu, Samuel (ECY; Ottaway, William (DEC; betsey.wingfield@ct.gov; Gloria.Post@dep.nj.gov; elizabeth.lewis-michl@health.ny.gov
Optional Attendees: Kavlock, Robert; Impellitteri, Christopher; Caporale, Cynthia; Fitz-James, Schatzi; Raffaele, Kathleen; Flowers, Lynn; Sinks, Tom; Orme-Zavaleta, Jennifer; Watkins, Tim; Buckley, Timothy; Sonich-Mullin, Cynthia; Gilliland, Alice; McDonald, James; Gettle, Jeaneanne; Carter, Bobbi; Behl, Betsy; Strong, Jamie; Foster, Stiven; Deener, Kathleen; Barber, Andrea; Scheuer, Amy; MARZ Nicole; Karoly, Cyndi; Mundrick, Doug; France, Danny; Walker, Mary; Zapata, Cesar; Allenbach, Becky; Heard, Anne; Lapierre, Kenneth; Shehee, Mina; Hall, Renea; Campbell-Dunbar, Shawneille; Mitchell, Ken; Jessica Godreau; Kemker, Carol; Dean, Glenda; Poolos, Ed; Harrison, Dennis; Hays, Lewis; Capp, James; Carnley, Keith; Booth, Elizabeth; Justin B. Green; Zimmerman, Jay; Kinard, Doug; Bird, Joel (ECY); Yaquian-Luna, Jose; Taylor, Dawn; Sassman, Hannah; Braverman, Carole; O'shea, Marie; Harris, Kimberly; Nwogu, Peter; Azzam, Nidal; Maddaloni, Mark; Cutt, Diana; mmaddalo22@gmail.com; Recer, Gregg M (HEALTH); Leach, James F (HEALTH); Deming, Justin H (HEALTH); Parsons, Patrick J (HEALTH); Spink, David C (HEALTH); Wu, Qian (HEALTH); Gwinn, Maureen; Pociu, Shannon; Flaherty, Colleen; Hauchman, Fred; Malone, Kevin M (HEALTH)

[PFAS Call notes May 22 2017.docx](#)
[PFAS Overview presentation Aug 7.pdf](#)
[ITRC PFAS Team Aug 7.pdf](#)

If you have not already done so, please register for today's webinar:

Personal Matters / Ex. 6

Presentation materials attached.

EPA-ECOS PFAS Call
August 7, 2017
4:00-5:00 pm ET

Conference Line / Ex. 6

Code

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The purpose of this call (every other month) is to share information on PFAS work, including analytical methods, toxicity and treatment.

Draft Agenda

Welcome and Introductions (Lisa Matthews, State Liaison, EPA ORD)

US EPA Cross-Agency Coordination of PFAS Activities (Bob Kavlock, Acting Assistant Administrator, EPA ORD)

Update on EPA PFAS Analytical Methods Workgroup (co-chairs: Chris Impellitteri, ORD; Cindy Caporale, Region 3; and Schatzi Fitz-James, OLEM)

Interstate Technology & Regulatory Council (ITRC) PFAS Team (Patricia Reyes, ITRC Director)

State Updates

Discussion (All)

Adjourn

Attachment:

May 22 call summary

Lisa Matthews

Senior Advisor and State Liaison

US EPA Office of Research and Development

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US EPA Cross-Agency Coordination of PFAS Activities

August 7, 2017

- Introduction to PFAS
- US EPA Cross-Agency Coordination
- Overview of US EPA PFAS Activities
- Additional Slides

- A class of man-made chemicals that are ubiquitous due to:
 - Wide variety of industrial and consumer uses
 - Not known to degrade in the environment
 - High mobility
- They are a concern due to:
 - Known or suspected toxicity, especially for PFOS and PFOA
 - Bioaccumulation
 - Can persist in humans for several years
 - Shorter PFAS tend to be highly mobile, longer PFAS less mobile
- Information on PFAS is rapidly evolving



Cross-Agency Coordination of PFAS Activities

- **PFAS coordination is led through EPA's Office of the Science Advisor**
- **PFAS is a cross-Agency issue, but also multifaceted:**
 - Human health toxicity
 - Exposure
 - Analytical methods
 - Risk management
 - Risk communication
- **Currently there are three cross-Agency workgroups:**
 - Human health toxicity
 - Analytical methods
 - Data quality
- **This broad array of issues requires coordination of each individual aspect, but also overarching coordination of all issues to ensure that the Agency has an awareness of all ongoing and proposed activities.** 4



Current PFAS Activities: OCSPP

- **EPA's New Chemicals Program**
 - Review hundreds of pre-market alternatives for PFOA and related chemicals since 2000 before they enter the marketplace.
- **Significant New Use Rule (SNUR)**
 - Proposed on January 21, 2015 to require manufacturers, importers, and processors of PFOA and related chemicals (including as part of articles), to notify EPA at least 90 days before starting or resuming new uses of these chemicals in any products.
 - Notification provides EPA opportunity to conduct risk assessment/management for the new use
- **PFOA Stewardship Program**
 - Eight companies participated in the program and successfully eliminated production of PFOA.
 - Designed to phase out PFOA and related per- and polyfluoroalkylated substances (PFAS) including potential PFOA precursors by these companies by the end of 2015.



Current PFAS Activities: OLEM

- **EPA Federal Facility Superfund Program**
 - Program is actively engaged in a PFAS cleanup process at 32 Federal Facility National Priorities List (NPL) sites.
 - It is anticipated that this number will grow since there are known or suspected contaminations of PFAS at many of the 140 DOD Federal Facility NPL Sites.
 - PFAS detections in groundwater range from non-detect (based on analytical method limitations) or slightly exceeding the Drinking Water Health Advisory of 70 parts per trillion (ppt; PFOA and PFOS combined) to 2,000,000 ppt.
 - Drinking water has been impacted at 17 of these Federal Facility NPL sites.
- **Office of Superfund Remediation and Technology Innovation (OSRTI)**
 - 14 known impacted non-Federal NPL sites, including one proposed for listing (St. Gobain Hoosick Falls, NY)
 - 100s potential NPL sites (e.g. 100 metal plating sites, 300 landfills)
- **Regional Assistance**
 - Holding site specific consultations with EPA regions on investigations of PFAS contamination



Current PFAS Activities: ORD

- **EPA has been studying exposure and health effects of PFAS for more than 15 years.**
- **Health Effects**
 - Compiling considerable knowledge on the toxicological effects of various PFAS, including studies on the fate of PFAS in the body
 - Conducting research to study the potential hazards of PFAS in the environment using computational toxicology modeling
- **Analytical Methods/Exposure Assessment**
 - Ongoing research on analytical methods, in collaboration with program and regional offices, for measurement of PFAS in environmental media
 - Evaluating sources, environmental fate and transport, and exposure to human and non-human receptors
- **Risk Assessment**
 - EPA's Provisional Peer-Reviewed Toxicity Value (PPRTV) program completed a health assessment for perfluorobutane sulfonate (PFBS), a substance similar to PFOA and PFOS, in 2014
 - EPA identified PFAS as a chemical class of interest to the Agency in the 2015 multi-year agenda for the Integrated Risk Information System (IRIS) program
- **Risk Management**
 - Characterize PFAS contamination in the soil, surface water and groundwater at military installations where aqueous film forming foams (AFFF) have been used extensively
 - With the Air Force Institute of Technology (AFIT), test in situ remediation technologies to remove PFAS at contaminated sites



Current PFAS Activities: OW

- **Published Drinking Water Health Advisories (HA) in 2016 for PFOA and PFOS**
 - HAs are non-regulatory information for federal, state and local officials to consider when addressing drinking water contamination.
 - Identified 0.07 µg/L (70 parts per trillion) as the HA level for PFOA and PFOS combined and provided information about treatment and monitoring.
- **Evaluating PFOA and PFOS for regulatory determination under the Safe Drinking Water Act (SDWA)**
 - PFOA and PFOS are on the fourth Contaminant Candidate List (CCL 4) published in November 2016. EPA's Office of Water is assessing PFOA and PFOS against the three SDWA regulatory determination criteria:
 - *May have an adverse effect on the health of persons*
 - *Is known to occur or there is a substantial likelihood that it will occur in public water systems with a frequency and at levels of public health concern*
 - *In the sole judgment of the Administrator, regulating the contaminant presents a meaningful opportunity for health risk reductions for persons served by public water systems*
 - EPA must decide whether or not to regulate at least five CCL4 contaminants by January 2021.
 - Preliminary regulatory determinations for public comment expected in 2019 (to enable final regulatory determinations by January 2021).



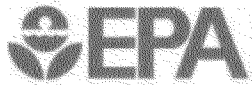
Current PFAS Activities: Regions

- **PFAS have been identified as an important issue in the EPA regions. Below are the general, ongoing efforts in the regions:**
 - Working collaboratively with states, local and federal partners, particularly DOD, to address concerns with PFAS contamination of public and private drinking water wells and legacy contamination at Superfund sites.
 - Providing support to states on different issues, including direct analytical support for sites, method improvement, method validation studies and quality assurance protocols.
 - Assisting states, local agencies and federal facilities with public messaging regarding risks.
 - Regions have had to issue Safe Drinking Water Act Administrative Orders to federal facilities (Naval Air Warfare Center, Warminster, PA, Naval Air Station Joint Reserve Base Willow Grove, Horsham, PA and Former Pease Air Force Base in Portsmouth, NH) in order to protect public supply wells given the emergent nature of this class of chemicals and the slow reaction time of other federal agencies.
- **Regional laboratory representatives participate in national and regional programmatic meetings offering technical advice with expertise in analytical methodology and quality acceptability.**

- **EPA ORD and the Office of Land and Emergency Management (OLEM) lead a cross-EPA workgroup on characterizing human health hazards**
 - To characterize the available toxicity information for approximately 30 PFAS of interest to various program offices or regions
 - To develop quantitative toxicity values for multiple PFAS, other than PFOA and PFOS
 - To inform evidence-based decisions by EPA offices and regions regarding potential human health risks from ongoing or future exposures

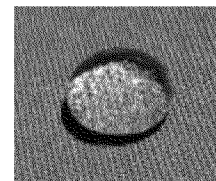
Category	Draft Final PFAS List	Acronym
Perfluoro carboxylic acids	Perfluorododecanoic acid	PFDoA
	Perfluoroundecanoic acid	PFUnA
	Perfluorodecanoic acid	PFDA
	Perfluorononanoic acid	PFNA
	Perfluorooctanoic acid	PFOA
	Perfluoroheptanoic acid	PFHpA
	Perfluorohexanoic acid	PFHxA
	Perfluoropentanoic acid	PFPeA
	Perfluorobutyric acid	PFBA
Perfluoro sulfonates	Perfluorodecanesulfonate	PFDS
	Perfluorononanesulfonate	PFNS
	Perfluorooctanesulfonate	PFOS
	Perfluoroheptanesulfonate	PFHpS
	Perfluorohexanesulfonate	PFHxS
	Perfluoropentansulfonate	PFPeS
	Perfluorobutanesulfonate	PFBS
Perfluoro sulfonamide	Perfluorooctanesulfonamide	PFOSA
Fluorotelomer sulfonates	Fluorotelomer sulfonate 8:2	FtS 8:2
	Fluorotelomer sulfonate 6:2	FtS 6:2
Perfluoro sulfonamidoacetic acids	N-ethyl-N-((heptadecafluorooctyl)sulfonyl)glycine	NEtFOSAA
	N-(Heptadecafluorooctylsulfonyl)-N-methylglycine	NMeFOSAA
Fluorotelomer alcohols	Fluorotelomer alcohol 8:2	FtOH 8:2
	Fluorotelomer alcohol 6:2	FtOH 6:2
Perfluoro ether carboxylic acids	Perfluoro(2-methyl-3-oxahexanoic) acid	GenX
	4,8-dioxa-3H-perfluorononanoic acid	ADONA
Fluorotelomer phosphates	6:2 Fluorotelomer phosphate monoester	6:2 monoPAP
	6:2 Fluorotelomer phosphate diester	6:2 diPAP
	8:2 Fluorotelomer phosphate monoester	8:2 monoPAP
	8:2 Fluorotelomer phosphate diester	8:2 diPAP
	6:2/8:2 Fluorotelomer phosphate diester	6:2/8:2 diPAP
Fluorotelomer carboxylic acid	5:3 Polyfluorinated acid	5:3 acid

- **OLEM/Region 3/ORD lead a cross-EPA workgroup on method development and validation**
 - To develop multi-laboratory validated methods for analyzing sample types other than drinking water (waters and solids) and quantifying 24 PFAS. Currently performing a multi-lab validation of a method for the 24 PFAS which was developed by the Region 5 Chicago Regional Lab
 - To develop sampling protocols to address PFAS analytical data quality issues Regions have identified
- **Region 10 and Region 3 lead a cross-EPA workgroup on evaluating data quality issues regions have identified**
 - To develop guidelines for data deliverables and assessment criteria



ADDITIONAL SLIDES

- Properties of PFAS range depending on carbon chain lengths and functional groups.
- PFAS generally occur as mixtures and are not well characterized.
- PFAS provide desirable performance because they repel both oil and water:
 - The fluorinated carbon tail is both lipophobic/oleophobic (repelled by fats and oils) and hydrophobic (repelled by water).
 - The functional group head can vary but is often hydrophilic (attracted to water).
- As a result of these unique surfactant properties and their stability, they are common surfactants and stain preventers.





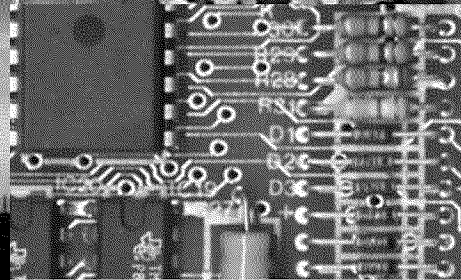
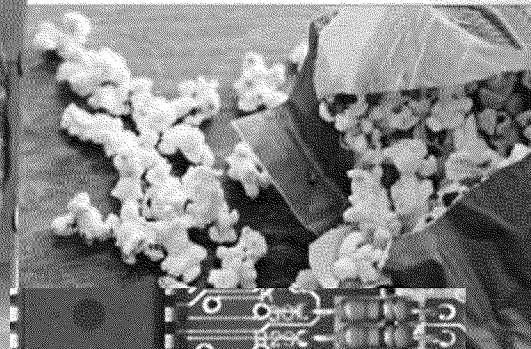
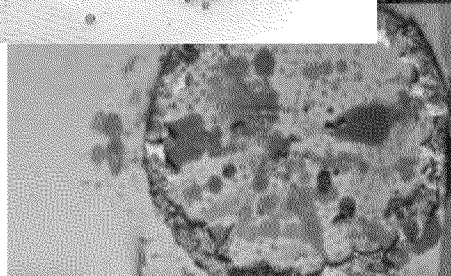
Production of PFAS

- PFAS production occurs by two primary production methods: Electrochemical Fluorination and Telomerization.
- During production of the intended products, many residuals and precursors are carried forward into the final formulations (e.g., FTOHs and PFOA may be found in fluoropolymers).
- Many PFAS are used as processing aids in production of other PFAS products. This results in:
 - Primary production facilities that synthesize PFAS chemicals, e.g. chemical plants
 - Secondary production facilities that produce products using PFAS, e.g. textile and paper facilities, fluorocarbon plastics production
- Industry is changing formulations in response to regulatory drivers and mounting toxicity and persistence data. However, replacement chemicals are unknown as to persistence, toxicity and bioaccumulation.

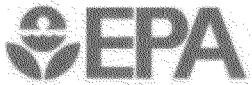


Uses of PFAS

- Food contact surfaces such as cookware¹, pizza boxes, fast food wrappers, popcorn bags, etc.
- Polishes, waxes and paints
- Stain repellants for carpets, clothing, upholstered furniture, etc.
- Cleaning products
- Dust suppression for chrome plating
- Electronics manufacturing
- Oil and mining for enhanced recovery
- Performance chemicals such as hydraulic fluid, fuel additives, etc.



¹ PFOA has been phased out, however there is little evidence that the chemicals that have replaced PFOA are much safer.



Sources of PFAS



- **Landfills and leachates from disposal of consumer and industrial products containing PFAS**
- **Land where wastewater treatment plant biosolids was applied**
 - Note: Biosolids applied following regulations should be protective to human exposure via ingestion of crops (Blaine et al. 2013 and 2014)
- **Direct release of PFAS products into the environment – such as use of aqueous film forming foam (AFFF) in training and emergency response**



Analytical Methods

- Only PFOS, PFOA and PFBS have vetted toxicity values at this time. Therefore, for initial investigations these would be the primary PFAS contaminants of concern.
 - Drinking Water: EPA Method 537 Version 1.1
 - Media other than drinking water: Each contract lab has their own method (most loosely based on EPA 537) since a standard HW method does not exist
- ORD, Region 5 and others are developing methods for PFAS precursors and PFAS in non-DW matrices (surface waters, groundwater, wastewater, biosolids, soils, sediments, etc).
- OLEM, OW, ORD, and Regional Labs currently conducting a multi-lab validation effort to establish an EPA method(s) for non-DW media.
- ORD and others are developing methods to identify unknown PFAS in environmental samples due to transformations, degradation, new formulations, etc.

To: Strynar, Mark[Strynar.Mark@epa.gov]; Lindstrom, Andrew[Lindstrom.Andrew@epa.gov]; Medina-Vera, Myriam[Medina-Vera.Myriam@epa.gov]; Biales, Adam[Biales.Adam@epa.gov]; Newton, Seth[Newton.Seth@epa.gov]; McCord, James[mccord.james@epa.gov]; Watkins, Tim[Watkins.Tim@epa.gov]; Orme-Zavaleta, Jennifer[Orme-Zavaleta.Jennifer@epa.gov]; Culpepper, Linda[linda.culpepper@ncdenr.gov]; Allenbach, Becky[Allenbach.Becky@epa.gov]; Smith, Emily J.[Smith.Emily@epa.gov]; Crofton, Kevin[Crofton.Kevin@epa.gov]; Guiseppi-Elie, Annette[Guiseppi-Elie.Annette@epa.gov]; Goode, Teresa[Goode.Teresa@epa.gov]; Oshima, Kevin[Oshima.Kevin@epa.gov]; Tong-Argao, Sania[Tong-Argao.Sania@epa.gov]; Hoffman, Brian[Hoffman.Brian@epa.gov]; Goldfarb, Steven[Goldfarb.Steve@epa.gov]; Grevatt, Peter[Grevatt.Peter@epa.gov]; Behl, Betsy[Behl.Betsy@epa.gov]; Henry, Tala[Henry.Tala@epa.gov]; Raffaele, Kathleen[raffaele.kathleen@epa.gov]; Sinks, Tom[Sinks.Tom@epa.gov]; Grimm, Ann[Grimm.Ann@epa.gov]; Kenneke, John[Kenneke.John@epa.gov]; Maguire, Megan[Maguire.Megan@epa.gov]; Hubbard, Carolyn[Hubbard.Carolyn@epa.gov]; Gilliland, Alice[Gilliland.Alice@epa.gov]; jordan.whichard@nc.gov[jordan.whichard@nc.gov]

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From: Buckley, Timothy

Sent: Thur 9/7/2017 12:39:02 PM

Subject: RE: Non-Targeted Lab Results Briefing to NC DEQ

[NC DEQ nontargeted results f2f RTP report08282017.pdf](#)

Now that our official report has been provided to NC DEQ and Region 4, I am able to share the presentation from our August 28th meeting. Thank you for your patience and understanding.

Tim Buckley

Timothy J. Buckley, PhD
Director of the Exposure Methods & Measurements Division
National Exposure Research Laboratory
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Research Triangle Park, NC 27711

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-----Original Appointment-----

From: Buckley, Timothy

Sent: Monday, August 14, 2017 2:19 PM

To: Buckley, Timothy; Strynar, Mark; Lindstrom, Andrew; Medina-Vera, Myriam; Biales, Adam; Newton, Seth; McCord, James; Watkins, Tim; Orme-Zavaleta, Jennifer; Culpepper, Linda; Allenbach, Becky; Smith, Emily J.; Crofton, Kevin; Guiseppi-Elie, Annette; Goode, Teresa; Oshima, Kevin; Tong-Argao, Sania; Hoffman, Brian; Goldfarb, Steven; Grevatt, Peter; Behl, Betsy; Henry, Tala; Raffaele, Kathleen; Sinks, Tom; Ann Grimm; Kenneke, John; Maguire, Megan; Carolyn Hubbard; Gilliland, Alice; jordan.whichard@nc.gov

Cc: Walker, Mary; Flaherty, Colleen; Johnson, Chris; Moore, Zack; Shehee, Mina; Aubee, Catherine; Risen, Amy J; Pritchett, Jamie R;

michael.devito@nih.gov; Cox, Heidi; Kritzer, Jamie; Zimmerman, Jay; Grzyb, Julie; Midgette, Robert; Holman, Sheila; McClain, Jennifer; Tiago, Joseph; Tricas, Marisa; Speth, Thomas; Burneson, Eric; Thompsons, Anita; Strong, Jamie; Satterwhite, Dana; Godreau, Jessica; Lincoln, Larry; Campbell-Dunbar, Shawneille; Staley, Danny; Kemker, Carol; Gettle, Jeaneanne; Adams, Glenn; Flowers, Lynn; Impellitteri, Christopher; Scott, Michael; Tarr, Jeremy M; Talley, Noelle S; Karoly, Cyndi; Gregson, Jim; Dittman, Elizabeth; Allen, Trent; Fenton, Suzanne (NIH/NIEHS) [E]; Carroll, Gregory; France, Danny; Mort, Sandra L; Grantham, Nancy; Christopher Lau; Munger, Bridget; Hines, Erin; Andrew Gillespie; Hall, Renea; Davis, Molly; Shell, Karrie-Jo; Schwartz, Paul; Bush, William; Mancusi-Ungaro, Philip; Janovitz, Sara; Ravenscroft, John (Ravenscroft.John@epa.gov); Tilson, Betsey; Gordon, Scott; Rubini, Suzanne; Detlef Knappe; Mattas-Curry, Lahne; Young, Sarah

Subject: Non-Targeted Lab Results Briefing to NC DEQ

When: Monday, August 28, 2017 9:00 AM-12:00 PM (UTC-05:00) Eastern Time (US & Canada).

Where: EPA RTP C111A-B; Agenda attached.

The primary goal of this briefing is to communicate lab results to NC DEQ and address their questions. Becky Allenbach in Region 4 and Linda Culpepper NC DEQ will extend invitation to others in their organization as appropriate. I am expanding invite list to include other labs and Centers and EPA Program Offices with potential interest.

A webinar link has been provided for remote access.

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Personal Matters / Ex. 6

Conference Number:

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Conference Code:

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NERL Report of Non-Targeted PFAS Results to NC DEQ

August 28, 2017

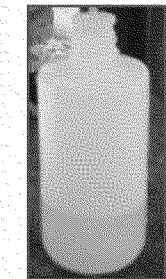
**U.S. EPA
Research Triangle Park, NC
Room C111-A/B**



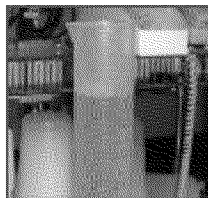
Introduction/Background

- NERL in collaboration with NCSU has been conducting PFAS research in the Cape Fear River for the last 10 years (Nakayama et al., 2007)
- Recent work based on non-targeted analysis identified a range of new PFAS (~15) from two broad families – Gen X and Nafion in Cape Fear and drinking water (Strynar et al., 2015)
- GenX was measured in drinking water mean conc. 631 ng/L (Sun et al., 2016)
- Local press picks up Sun et al., 2016 findings
- NC DEQ, R4, & NERL partner to monitor effectiveness of source remediation
- NC DEQ conducts sampling in Cape Fear over 8 weeks at 13 locations including Chemours outfall, upstream, down stream, well, source, drinking water
- NERL has provided three prior reports giving GenX results
- Today is the first report that includes non-targeted analyte results

Sample Processing Nakayama et al., 2009



1 L HDPE bottles
5 mL 1:1 HNO₃ (35%):DI
Shipped ambient



Pour water out
of sample
bottle for
volume
measurement



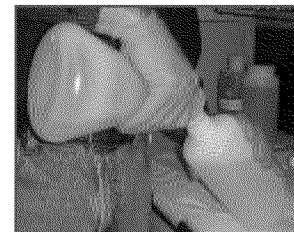
Wash bottle with 10
mL MeOH, add water
back to bottle, add IS
Shake



Filter entire contents
Whatman GF/A 1.7 um

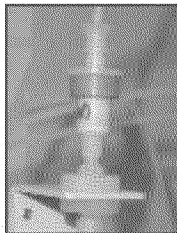
All samples
Treated same
way

- Trip Spike
- Blanks
- Unknowns
- Calibration

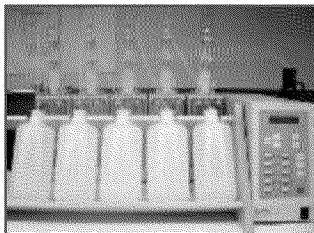


Add filtered water back into
original bottle

Subsample 500 mL
Store 500 mL

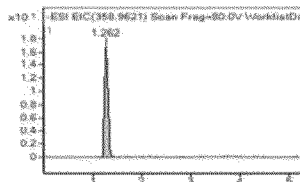


Load onto SPE tube
Waters Plus style WAX

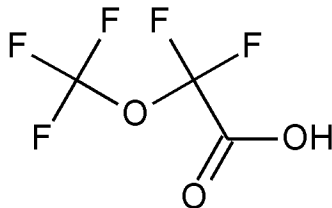


Non-Targeted Methods

- High resolution mass spectrometry allows one to observe an unknown compound as a peak in a chromatogram and to ultimately predict the identity of this unknown
- Initially, the mass spectrometer assigns a mass for each peak observed, for example 179.9846 Daltons (Da)

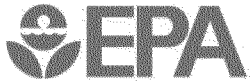


- Software then calculates the exact number and type of atoms needed to achieve that measured mass, example $C_3HF_5O_3$ (need this number and type of atoms to weigh this much)
- Software and fragmentation experiments allow determination of most likely structure:



Molecular Formula: $C_3HF_5O_3$
 Monoisotopic Mass: 179.984585 Da
 [M-H]⁻: 178.977308 Da

- With mass, formula, and structure determined, identity can be assigned by searching against databases of known compounds, example CAS number 674-13-5
- Search for standards from commercial sources to confirm identification if possible



Estimating NTA Analyte Concentration

$$[\text{NTA}] = \frac{[\text{GenX}] \cdot \text{NTA}_{\text{PA}}}{\text{GenX}_{\text{PA}}}$$

Where: **[NTA]** is the concentration of the non-targeted analysis analyte (ng/L)

[GenX] is the concentration of **GenX** (ng/L)

NTA_{PA} is the integrated peak area for the non-targeted analysis analyte

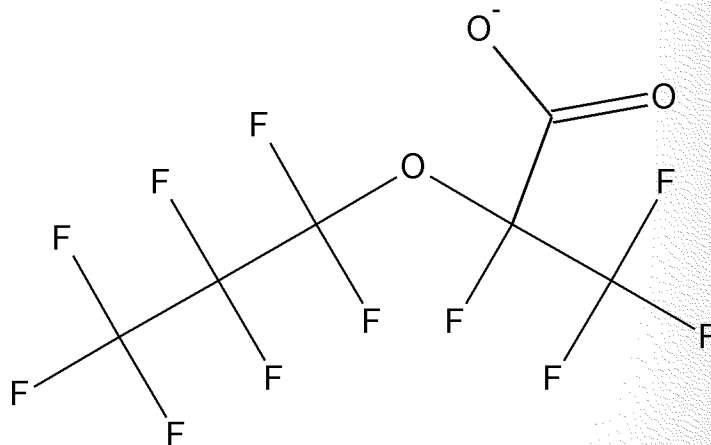
GenX_{PA} is the integrated peak area for **GenX**



Non-Targeted Analytes (NTA) Measured by LC/TOFMS Analysis

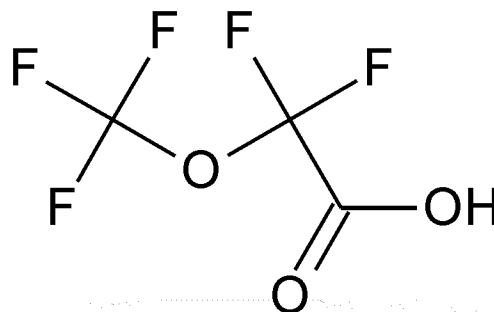
Short Name	Chemical Name	Formula	CAS no.	Monoisotopic Mass (Da)
Nafion Byproduct 1	Unknown	$C_7HF_{13}O_5S$	66796-30-3	443.9337
Nafion Byproduct 2	Unknown	$C_7H_2F_{14}O_5S$	749836-20-2	463.9399
GenX	2,3,3,3-Tetrafluoro-2-(heptafluoropropoxy)propanoic acid	$C_6HF_{11}O_3$	13252-13-6	329.9750
PFMOAA	(2,2-difluoro-2-(trifluoromethoxy)acetic acid)	$C_3HF_5O_3$	674-13-5	179.9846
PFO2HxA	perfluoro-3,5-dioxahexanoic acid	$C_4HF_7O_4$	39492-88-1	245.9763
PFO3OA	perfluoro-3,5,7-trioxaoctanoic acid	$C_5HF_9O_5$	39492-89-2	311.9680

- Class: PFECAs
- Formula: $C_6HF_{11}O_3$
- CAS no.: 13252-13-6
- Molecular Mass: 329.9750 Da
- Ref: Strynar et al., ES&T 2015;
Sun et al., 2016



PFMOAA :
(2,2-difluoro-2-(trifluoromethoxy)acetic acid)

- Class: PFECAs
- Formula: $C_3HF_5O_3$
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